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14. ABSTRACT

Despite considerable progress made in computational fluid mechanics, chemical kinetics and soot processes in recent years, the study of complex fuels in gas turbine engines, including soot processes is still a daunting task and will remain so for the foreseeable future. Traditionally, the combustion community has chosen either to focus on the fluid mechanics of real engines with simplified chemical kinetics or to study simple laminar flames with detailed kinetics and transport. This dichotomy is a necessity as the level of computer power needed to solve the complete engine/chemistry problem will not be available for years to come. The challenge is even greater, to the point of being unrealistic, if complex fuels and soot are to be included. Our research program has the realistic objective of examining the structure of gaseous laminar diffusion flames perturbed by the addition of a few thousand ppm of complex fuels such as: higher alkanes and aromatics, their combination in jet fuel surrogates and, ultimately jet fuel itself. The aim is to study their flame structure and soot behavior in the entire pressure range of relevance to modern gas turbines, that is, 1-40 atm. A counterflow diffusion flame is selected as an optimal environment for the research due to the suppression of buoyancy instabilities that typically plague coflow flames at high pressures, the unparalleled level of control that it provides on the soot formation process, and the opportunity of modeling the system as one-dimensional, which is advantageous for fuels with a very large chemical mechanism, such as JP-8.

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COMPUTATIONAL AND EXPERIMENTAL STUDY OF THE STRUCTURE OF DIFFUSION FLAMES OF JET FUEL AND ITS SURROGATES AT PRESSURES UP TO 40 ATM

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Status of Effort/Objectives

Despite considerable progress made in computational fluid mechanics, chemical kinetics and soot processes in recent years, the study of complex fuels in gas turbine engines, including soot processes is still a daunting task and will remain so for the foreseeable future. Traditionally, in the case of simple fuels, the combustion community has chosen either to focus on the fluid mechanics of real engines with simplified chemical kinetics or to study simple laminar flames with detailed kinetics and transport. This dichotomy is a necessity as the level of computer power needed to solve the complete engine/chemistry problem will not be available for years to come. The challenge is even greater, to the point of being unrealistic, if complex fuels and soot are to be included. Our research program has the realistic objective of examining the structure of gaseous laminar diffusion flames perturbed by the addition of a few thousand ppm of complex fuels such as: higher alkanes and aromatics, their combination in jet fuel surrogates and, ultimately jet fuel itself. The ultimate goal is to study their flame structure and, possibly, soot behavior in the entire pressure range of relevance to modern gas turbines, that is, 1-40 atm.

Accomplishments/New Findings:

Research in the prior funding periods was focused on a balanced experimental and computational approach on both counterflow and coflow laminar diffusion flames. The former offer one of the most elementary fluid mechanic scenarios resulting in a one-dimensional flow field. It is the first order of business when tackling complex chemistry, such as that of jet fuel, its surrogates and the surrogate components, including, eventually, soot formation. It is also an ideal scenario to test high-pressure effects to values of relevance to modern gas turbines (up to 40 atm), as further explained below. The coflow laminar flames add the additional complexity of a two-dimensional flow field and consequently represent a more challenging benchmark to validate the computational approach, especially with respect to the incorporation of reduced kinetics. In both counterflow and coflow scenarios, experimental and computational work are intertwined to make progress in the field in unison. As a result of this coordinated activity, eight peer-reviewed articles [1-8] were published and a number of presentations were given at national and international meetings. Principal results will be discussed below.

Counterflow Laminar Diffusion Flames Doped with Jet Fuel, its Surrogates and their Components

Principal results are reported in Refs. [1-3] and [7-8]. Here we summarize key points and, most importantly, we provide a glimpse of the modus operandi and the rationale behind it. A counterflow diffusion flame is selected as an optimal environment for the research due to the suppression of buoyancy instabilities that typically plague coflow flames, especially at high pressures, the opportunity of modeling the system as one-dimensional, which is advantageous for fuels with a very large chemical mechanism, such as JP-8, its surrogates and reference fuel components, and the unparalleled level of control that it provides on the soot formation process.

Gaseous flames of either methane or ethylene provide a base line. They are treated essentially as "flow reactors" with well defined temperature time-histories. A variety of liquid fuels are then prevaporized and introduced in such environments either individually or in combination as a perturbation of the baseline flames, at concentrations not exceeding a few thousand ppm. Whereas the approach is not intended to be as well controlled as traditional chemistry tools, such as flow reactors or shock tubes, it adds the critically important complexity of transport-chemistry interaction in the simplest possible flames. As such, it is an inevitable intermediate step in the study of the combustion of complex fuels before the investigation of turbulent counterparts.

With respect to fuels tested, in addition to Jet Fuel, we have used a number of surrogates including: the two-component Aachen surrogate [9], the six-component Utah surrogate [10] and, recently, the three-component Princeton surrogate [11]. The "ideal" surrogate depends on the properties of the jet fuel that the surrogate is intended to capture. However, to develop a database of broad interest to the combustion community, we have focused also on individual key ingredients appearing in most, if not all, surrogates, including: higher alkanes (n-decane, n-dodecane, n-tetradecane, iso-octane), some cyclic compounds (methyl-cylcohexane), and some aromatics (toluene, m-xylene, 1,2,4-trimethylbenzene, tetralin). They are used either individually [7-8] or in combination. As a result, the experimental and computational tools that we have developed thus far present a unique infrastructure for the testing of complex fuels in simple flames, regardless of the surrogate formulation.

To span a sufficiently broad range of conditions, we focused first on an ethylene counterflow diffusion flame doped with 2000 ppm on a molar basis of either jet fuel or three jet fuel surrogates under incipient sooting conditions [1]. We refer to it as the Incipiently Sooting Flame (ISF). The doped flames have identical stoichiometric mixture fractions (z_f = 0.18) and strain rates (a= 92 s^{-1}), resulting in a well-defined and fixed temperature/time history for all. By selecting this composition, conditions conducive to incipient soot formation are analyzed and the flame is positioned on the oxidizer side of the stagnation plane, as typical of hydrocarbon/air combustion. We also examined a baseline blue methane flame with a stoichiometric mixture fraction of 0.76, which for the purpose of this discussion, we refer to as the Blue Flame (BF) [2-3]. Also, these flames are doped with 1000 ppm (molar) of either jet fuel or jet fuel surrogates. This second set of flames provides a glimpse of the pyrolysis and oxidation behavior of jet fuel in a diffusion flame positioned on the *fuel* side of the gas stagnation plane and is representative of conditions that could be encountered in oxy-fuel combustion. These two flame scenarios span

a broad range of conditions, with a more pronounced role of the leakage of oxidative species through the flame in the second set of flames as compared to the first.

The chemical structure of all these flames was analyzed experimentally, by gas sampling via quartz microprobes and subsequent GC/MS analysis, and computationally using a semi-detailed kinetic mechanism for the surrogate blend that was provided by the group of Professor Ranzi in Milan with which we have been collaborating, or other mechanisms available in the literature [7-8]. Our findings suggest that the initial oxidation of jet-fuel is consistent with anticipated chemical kinetic behavior, based on thermal decomposition of large alkanes to smaller and smaller fragments and the survival of ring-stabilized aromatics at higher temperatures. Computationally, the one-dimensional code adopted a semi-detailed kinetic mechanism for the surrogate blend that is based on an existing hierarchically-constructed kinetic model for alkanes and simple aromatics, extended to account for the presence of tetralin and methylcyclohexane as reference fuels. The computational results are in reasonably good agreement with the experimental ones for the surrogate behavior, with the greatest discrepancy in the concentrations of aromatics. Good agreement between jet fuel and the surrogates is found with respect to critical soot precursors such as benzene and toluene in the ISF. Although the 6-component Utah/Yale surrogate performs better than the Aachen surrogate, the latter performs adequately and retains the advantage of simplicity, since it consists of only two components.

As an additional demonstration of the usefulness of the infrastucture we have in place, we tested the 3-component Princeton surrogate [11] experimentally and computationally, with results being presently analyzed. Figure 1 shows experimental and computational profiles of key species monitored in the flames that are reflective primarily of the dopant chemistry, as opposed to the underlying chemistry of the baseline flames. The top row pertains to the high-z_f methane Blue Flame (BF) and the bottom row to the low-z_f ethylene Incipiently Sooting Flame (ISF). In comparing the experiments with the computation, we notice that the pyrolysis of the surrogate components (left column) occurs at a slower rate in the model as compared to the experiments in both flames. The discrepancy is more pronounced in the methane flame. If we recall that the two flames are positioned on opposite sides of the stagnation plane, a tentative culprit might be the role of *oxidative* pyrolysis, due to trace species leaking through the flame, that should be more significant in BF as opposed to ISF, since in that case the flame is on the fuel side of the stagnation plane. Turning to the second set of compounds (middle column), the shift in the misalignment between predictions and measurements of the alkene is a direct consequence of the slower decomposition kinetics of decane in the model. Also, the concentrations are underpredicted in BF and overpredicted in ISF. In the case of cyclopentadiene, an intermediate of toluene pyrolysis, the model performs reasonably well in both flames. Lastly, an examination of some of the aromatics show that the model captures well benzene from toluene decomposition in BF, but underpredicts styrene and ethylbenzene. The situation is reversed in ISF, the sooting flame where they matter the most, in which the model invariably overpredicts these aromatic concentrations.
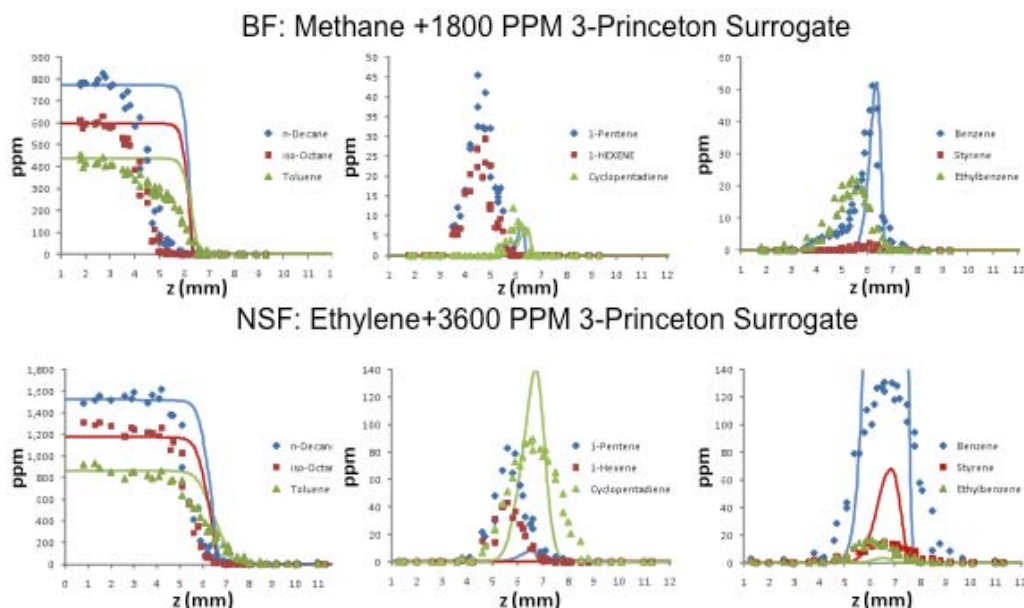
Figure 1: Example of application of our experimental and computational approach to the three-component Princeton surrogate. See text for details.

Two articles on the synergistic effects or lack there of in the chemistry of the studied surrogates are in preparation. As an indication of the insight on the chemical kinetics of complex fuels that can be gathered from our approach, we now briefly review completed studies on the individual reference fuel components, with a focus on Toluene [7] and 1,2,4-timethyl benzene (TMB) [8]. Profiles of critical toluene pyrolysis products and stable soot precursors were compared with computational models using two semi-detailed chemical mechanisms, one from Ranzi's group and another developed by the group of Professor Dryer in Princeton. Results show that in the methane flame some oxygen containing radicals like O and OH are contributing early on to the toluene destruction path. In the incipiently sooting ethylene flame, the primary attack is from H alone. This confirms the different challenges such flames pose to the validation of a chemical kinetic mechanism. The onset of toluene decay in these flames begins at relatively modest temperatures, on the order of 800 K. This reactivity is captured reasonably well by both chemical mechanisms in the methane flame, in the absence of reactants larger than C2 but not so in the ethylene flame, in the presence of a richer, more complex mixture. The aromatic ring opening mechanisms are not adequately modeled in either case. This discrepancy has implications for the modeling of practically relevant fuel blends with both aliphatic and aromatic compounds. The dominant species larger than toluene in the doped methane flame is ethylbenzene, which at least one of the mechanisms reproduces quite well. The largest measured species in the incipiently sooting flame is indene, whose concentration increases due to toluene addition is properly captured by one of the models. The experimental dataset reported here may help identifying future improvements to chemical kinetic mechanisms and complement other reactor datasets lacking the coupling of kinetics and transport of flame environments.

Turning to the second fuel component, TMB, experimentally we observed that because of the presence of aliphatic fragments TMB reactivity is enhanced in these flames with the onset of TMB decay beginning at relatively modest temperatures, on the order of 800 K [7]. The dominant path to stable species is driven by H radical attack and it leads in sequence to xylenes,

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toluene (through benzyl radical) and benzene formation. This enhanced reactivity is captured reasonably well by the model in the methane flame, but not in the ethylene flame, in the presence of a richer, more complex mixture. The model does not reproduce accurately the pathway yielding C3 and some C4 species from TMB cracking. Aromatic ring opening is the bottleneck in the TMB cracking process in the methane flame but not in the ethylene one. Indene, an important soot precursor for monoaromatic fuels since the second aromatic ring formation is considered to be a bottleneck in the process, is measured in the ethylene flame in poor agreement with the model predictions. The dataset presented here and available supplemental materials online may help in identifying improvements to the chemical kinetic mechanism of this reference fuel. Articles are in preparation on two additional reference fuel components: decane and iso-octane.

High-Pressure Counterflow Flames

With the joint support of AFOSR and NSF an experimental system was designed, fabricated and tested to stabilize steady diffusion flames at elevated pressures, up to 40 atm. In contrast with the much more common coflow configuration, the counterflow one is advantageous for the suppression of buoyancy instabilities that typically plague coflow flames at high pressures [12]. We review briefly key aspects of the progress to date to set the stage for the proposed work.

Counterflow burner developments

A high-pressure counterflow experimental setup was designed to reach 40 atm and was successfully tested at pressures as large as 30 atm, resulting in the establishment of either blue flames or marginally sooting ones. Above 15 atm., the replacement of nitrogen with helium as inert was found to be necessary to stabilize flames of good quality with respect to steadiness, laminarity, adiabaticity, one-dimensionality and acceptable flame thickness [12]. After going through scaling arguments, we demonstrated that the counterflow configuration is the *only* laminar flame that allows for the establishment of high-pressure, steady, adiabatic laminar flames. Although coflow flames at similarly high pressures have been stabilized [e.g., 13], they must be kept short to avoid buoynacy-induced instabilities. As a result, they are vitiated by heat/mass losses that make them problematic for computational modeling. The appearance of a sample flame at 30 atm is shown in Fig. 2. We show this photo as evidence of good soot control: the challenge at high pressures is not having a sooty flame, which high pressures favor, but producing soot in a highly controlled manned to be able to focus on the particle inception stage. This is one of the objectives of the present proposal.

Figure 2: 30-atm helium-diluted flame with helium as shroud gas.
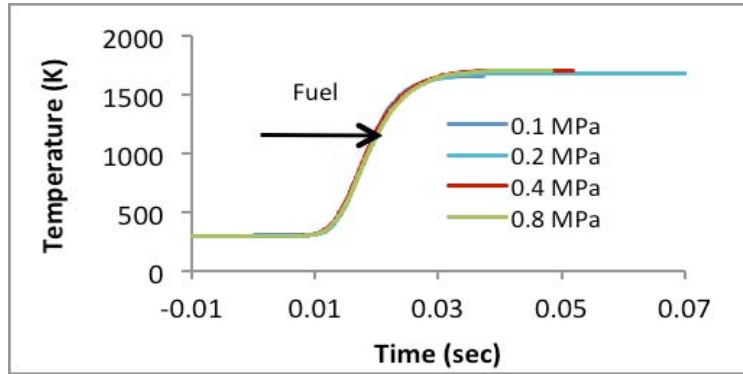
Figure 3: Computed temperature-time history as a function of pressure in flames with the same composition and strain rate

Gas sampling and GC/MS analysis

We summarize here some experimental/computational results to demonstrate our capabilities, albeit in a limited pressure range for the moment. We analyzed five flames at pressures ranging from atmospheric to 1.6MPa, in the high-pressure counterpart of what we have been doing at atmospheric pressure for some time [e.g., 14-16]. For space limitations we report selected results only in the 0.1-0.8 MPa range. The lower pressure flames are blue, whereas the 0.8 MPa flame has some faint soot luminosity at the center as detected by off plane visual observation. The flames have virtually identical composition and strain rate, with fuel mass fraction, stoichiometric mixture fraction and global strain rate at Y_f=0.12, Z_{st}=0.41 and a=57/s, respectively. The only difference is the pressure level and the overall mass flow rates, that for the flames to maintain a constant strain rate scale linearly with pressure. Figure 3 shows the computed temperature-time history for these flames. Modest differences are present in the peak temperature that could be offset by minor adjustments in inert concentrations. This plot exemplifies the capability of using the flame as a well-controlled flow reactor, with well-defined and fixed temperature-time history. The latter is crucial in soot formation and having a good control on it will enable us to isolate specific effects, such as fuel dependence, pressure, etc.

As to the sampling technique, one is often concerned with the intrusiveness of inserting the quartz microprobe into the flame. In this respect, we demonstrated in the scanning of flames in the 0.1-0.8 MPa that decreasing the size of the probe by taking into consideration the pressure-dependent flame thickness, $\delta_{diff} = \sqrt{\dfrac{D_{therm}}{a}\dfrac{p_0}{p}}$, where p is the pressure, subscript 0 refers to atmospheric conditions and D_{therm} is the thermal diffusivity, results in no deterioration of the resolution and good agreement with the computational model. Table 1 shows the dimensions of the probe used in these multiple scans. On the other hand, a scan at 1.6 MPa with a 100/40 μm (O.D./I.D.) probe showed a deterioration of spatial resolution.

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Table 1

Pressure (MPa)	0.1	0.2	0.4	0.8
I.D. (μm)	150	150	40	40
O.D. (μm)	360	360	150	150

Figure 4 shows some critical species for soot formation, as detected in an ethylene flame operated up to 8 atmospheres. The fuel is issued from the right and the origin of the abscissa is at the blue layer associated with flame chemiluminescence. Black, red, yellow and blue pertain to data for the 0.1, 0.2, 0.4 and 0.8 MPa, respectively. The continuous curves are generated by a computational model with detailed kinetics and transport using the Wang mechanism [17]. We show results for C_2H_2, Propyne and Allene, and C6-C9 growth species to give a flavor of the current capabilities. We observed that as the pressure is increased:

  i.   The flame gets progressively thinner, as expected;
 ii.   Major species (not shown) are in very good agreement with the computational model predictions;
iii.   Alkanes and alkenes decrease as pressure is increased, acetylene is relatively unchanged;
 iv.   C6-C9 Aromatics (and cyclic compounds) systematically increase, which correlates with the onset of soot; and
  v.   The computational results for C_6H_6 substantially underpredict its concentration.

This type of information provides insight into the necessary tweaking of chemistry models to bring about agreement with the measurements.

Development of the soot sampling procedure

Laser light extinction is generally not sufficiently sensitive for soot measurements in lightly loaded flames. The problem is exacerbated here since, to maintain a modest burning rate at high pressure, our flames are small, which implies that the optic path of the laser light in the sooting region is less than one cm. We thus explored thermophoretic sampling to measure particle size distribution and study soot morphology [18]. Lee et al. [19] showed in a coflow flame that sampling by quick insertion and retraction of a TEM grid produces large flow perturbations and a certain degree of mixing, resulting in poor spatial sampling resolution. By increasing the rigidity of the probe and reducing the flow perturbation, they were able to detect the soot growth along the flame, with better control as compared to the perturbed case. However, in the coflow flames adopted in [18] and [19], sampling locations are on the order of a few millimeters apart, which makes their approach incompatible with the present flames whose overall soot layer thickness is on the order of one mm, and decreases as pressure increases as $p^{-1/2}$. Thus, a much better spatial resolution is required.
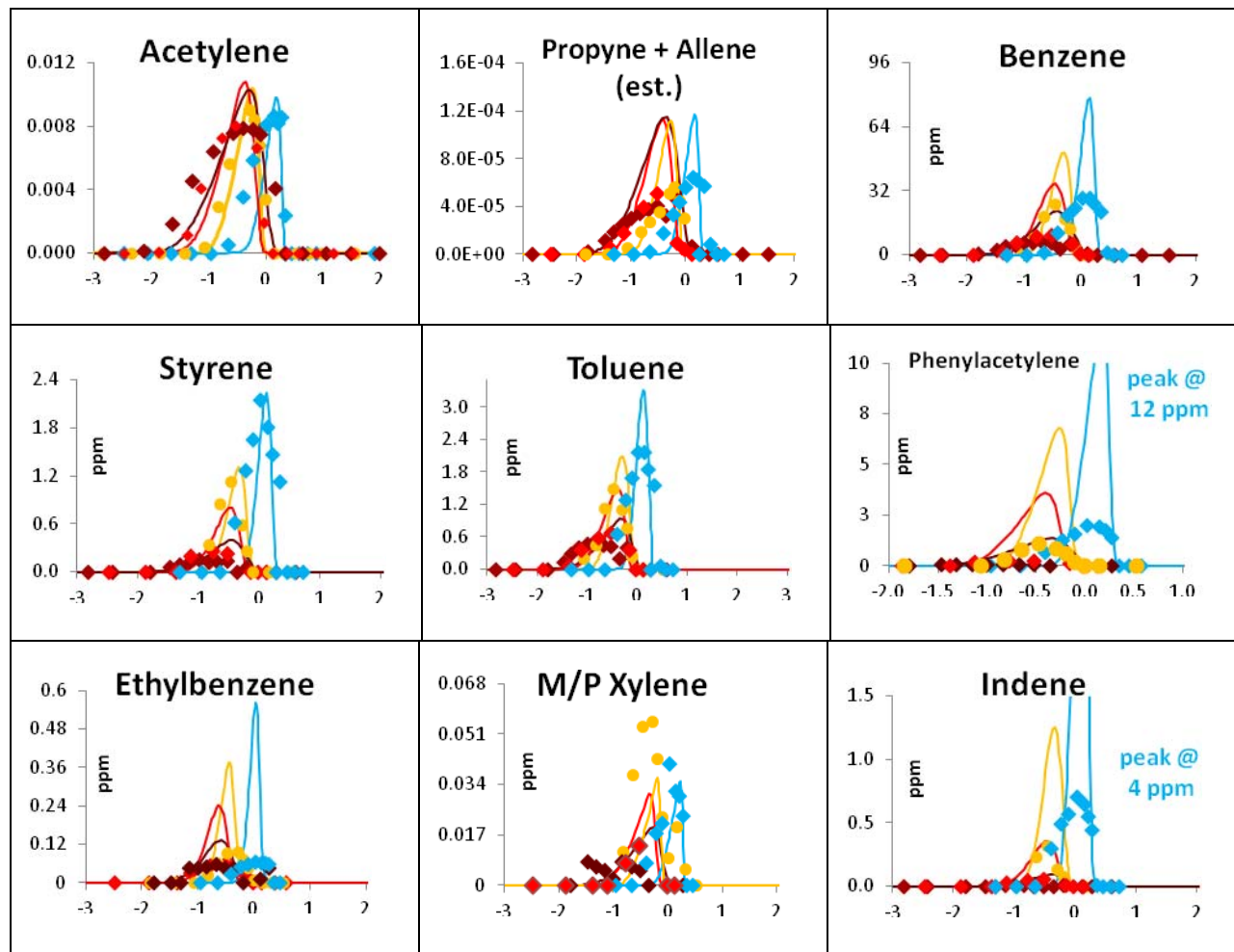
Figure 4: Mole fractions (ppm were specified) of some critical species in soot formation versus the relative position of the sampling probe with respect to the flame chmiluminescence layer. Fuel is issued from the left. Color-coded pressure legenda: 0.1, 0.2, 0.4, 0.8 MPa

To this end, we used the same 13.5 μm SiC wire that had been employed for temperature measurements via thin filament pyrometry [20], which produces minimal perturbation to the flame structure in view of the very small wire dimensions. The deposition of soot particles on the SiC wire needs to be limited in order to avoid the formation of a uniform, continuous coating, discern size and count individual particles. A pneumatic actuator located within the pressure chamber quickly inserted and retracted a fork carrying the SiC wire with a minimum residence time of 30msec. To avoid vibration of the wire within the soot layer, a rigid fork was attached to a horizontal sliding rail. Both were placed in a plane beneath the flame, to avoid any disturbance to the flow field, and the wire was attached to two small vertical extensions anchored on the fork. Finally, a screen was mounted above the fork for improved screening of the flame. The resulting setup, shown in Fig. 5 was successfully used to probe the soot layer with high spatial resolution.

The distance of the sampling points across the soot layer is computed by knowledge of the angle between the wire and the soot layer (or flame). A high-speed camera was used to measure the settling time of the wire after insertion, confirming that after a time comprised between 10 and 20 msec the wire stopped oscillating. This settling time is sufficiently short to yield good spatial resolution of soot sampling for exposure times on the order of tens of msec.
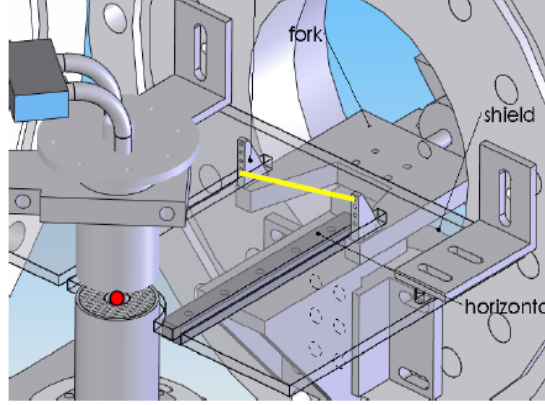

Figure 5: Setup for thermophoretic sampling as viewed from inside the chamber. The wire (yellow line) is tilted so as to sample the whole soot layer at once.

SEM images of the soot particles deposited on the wire are used to compute average size as a function of the position along the wire. To test our approach we sampled soot from ethylene-nitrogen flames, $Y_f = 0.212, Z_{st} = 0.4, a = 60/s, P = 1$ atm, where a is the strain rate, with a wire exposure time of 150msec. The average particle size is shown in Fig. 6. The SEM analysis does not detect particles below 5nm diameter because of the low contrast between particles and wire. To orient the reader, the steepest slope in the data in Fig. 6 is on the oxidizer side. The uncertainty of size measurement is ±15%. Similar, spatially resolved soot measurements were obtained at 30 atm. The size distribution in these measurements was monomodal, unlike the reported results from transparent and only particles on its edge can transmit the electron beam. In
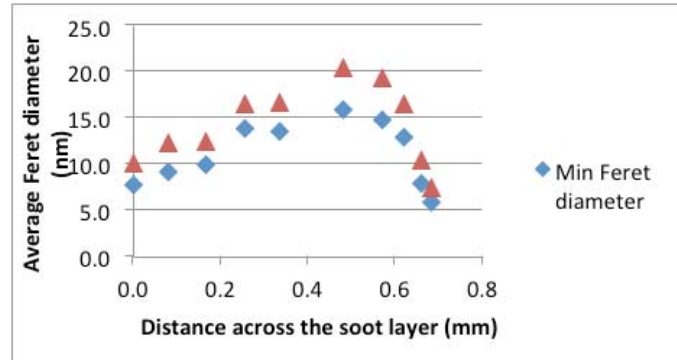
Figure 6: Average diameter of soot particles as a function of the distance across the soot layer. Fuel inlet on the left of the abscissa.

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Fig. 7 the wire appears as a dark area on the right while particles are visible on the edge; the two dark lines on the top and bottom left corners are the edges of the lacey carbon film. Figures 8 and 9 present two different particles, one with an amorphous structure, the other with a graphitic structure. In both cases the contact angle between soot particles and the wire suggest a liquid-like nature of the incipient sooting particles, also observed by other groups, with AFM analysis [21] and TEM diagnostics [22]. It is not clear if the graphitic structure of the particle in Fig. 9 is the result of carbonization while the particles sit on the wire, and changes in its internal structure are triggered by the hot environment. Tests need to be conducted for different wire residence times to check for experimental artifacts. These experiments and the resolved spatial profiles in Fig. 7 bode well for the extraction of quantitative data at high pressure. They confirmed the unprecedented level of control achieved in these diffusion flames. In conclusion, the soot sampling appears to be capable of resolving the soot layer spatially and of providing structural information of nascent soot particles.
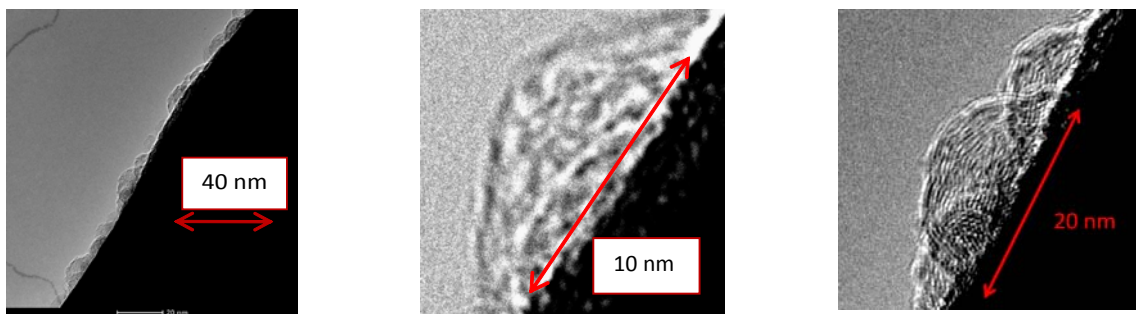
Figure 7: TEM image of the wire. **Figure 8:** Amorphous soot particle. **Figure 9:** Graphitic soot particle.

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Publications:

1. Jahangirian, S., McEnally, C. S., and Gomez, A., "Experimental Study of Ethylene Counterflow Diffusion Flames Perturbed by Trace Amounts of Jet Fuel and Jet Fuel Surrogates under Incipiently Sooting Conditions," *Combust. Flame* **156**:1799-1809 (2009).
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8. Carbone, F., Gomez, A. (2013) "Chemical Effects Of 1,2,4-Trimethyl Benzene Addition" to appear in the *Proceedings of the Combustion Institute,* vol. 3.

Meetings and Presentations:

a. 32nd International Combustion Symposium, Montreal, Canada, August 2008
b. Fuels Summit, NIST, Gaithersburg, MD, September 2008
c. AIAA ASM, Orlando, Florida, January 2009
d. U. S. Combustion Meeting, Ann Arbor, Michigan, May 2009
e. Fuels Summit Meeting, USC, Los Angeles, California, September 2009
f. Eastern States Section Meeting, University of Maryland, October 2009

g. AIAA ASM, Orlando, Florida, January 2010
h. 33rd International Combustion Symposium, Beijing, China, August 2010
i. Fuels Summit Meeting, Princeton University, September 2010
j. AIAA ASM Meeting, Orlando, Florida, January 2011
k. U.S. Combustion Meeting, Atlanta, Georgia, March 2011
l. Numerical Combustion Meeting, Corfu, Greece, April 2011
m. Eastern States Section Meeting, University of Connecticut, October 2011
n. 34th International Combustion Symposium, Warsaw, Poland, August 2012

Honors/Awards:

a. Program Co-Chair, 32nd International Combustion Symposium, Montreal, Canada (M. D. Smooke, 2008)
b. Fellow, AIAA (M. D. Smooke, 2009)
c. Fellow, SIAM (M. D. Smooke, 2010)
d. Combustion Institute Zeldovich Gold Medal (M. D. Smooke, 2012)